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TITLE: Method for identifying and synthesizing high dielectric

constant perovskites

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APPL-NO: 10/ 185432 [PALM] DATE FILED: June 28, 2002

RELATED-US-APPL-DATA:

Application 10/185432 is a continuation-in-part-of US application 09/300869, filed April 28, 1999, ABANDONED

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REPRESENTATIVE-FIGURES: NONE

ABSTRACT:

A method for forming stable structures which includes identifying compositions having a high probability of forming stable structures using predictive modeling and synthesizing the compositions under high pressure and high temperature conditions to form the stable structures. Preferred stable structures are perovskites having a three-dimensional framework of corner-linked MX.sub.6 octahedra. The predictive modeling allows evaluation of structural stabilities of given compositions while providing hypothetical molar volumes.

It also estimates the molecular polarizability of the compositions from the atomic polarizabilities of its constituent ions. The predictive modeling also calculates the relative dielectric constant of the stable structures using the Clausius-Mossotti relationship and selects compositions having combinations of ions with complimentary ionic radii and bonding preferences. The synthesis of the identified compositions is carried out using high temperature and high pressure techniques to induce a structural transition of the composition to a denser phase.

[0001] This application is a continuation-in-part of U.S. patent application Ser. No. 09/300,869, filed on Apr. 28, 1999.

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